Cotinine

Other names:	(-)-cotinine
	(S)-cotinine
	1-Methyl-5-(3-pyridinyl)-2-pyrrolidinone
	1-methyl-5-(3-pyridinyl)-(S)-2-pyrrolidinone
	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)-
	S-(-)-Cotinine
Inchi:	InChI=1S/C10H12N2O/c1-12-9(4-5-10(12)13)8-3-2-6-11-7-8/h2-3,6-7,9H,4-5H2,1H3
InchiKey:	UIKROCXWUNQSPJ-UHFFFAOYSA-N
Formula:	C10H12N2O
SMILES:	CN1C(=O)CCC1c1cccnc1
Mol. weight [g/mol]:	176.22
CAS:	486-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.375		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
rinpol	1740.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	619.20	K	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	14.95	kPa	537.70	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

pvap	19.90	kPa	548.40	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	29.82	kPa	564.20	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	49.74	kPa	585.60	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	69.56	kPa	601.30	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	79.50	kPa	607.40	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	101.32	kPa	619.20	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	197.04	kPa	655.40	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	247.52	kPa	669.70	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.20	K	20.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry:	https://www.doi.org/10.1016/j.tca.2014.08.033
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C486566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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